

# Stochastic Models and Monte Carlo Methods in Numerical Mathematics and Mathematical Physics

## Abstract.

Stochastic models serve nowadays as a powerful instrument for studying the dynamics of processes in natural and life sciences, in the broad spectrum, from simple models of financial mathematics in the form of systems of stochastic differential equations, to very complicated turbulence models involving PDE's whose parameters are random fields, governing the movement of energy spectrum from smallest viscous scales to large energy-containing vortices in the boundary-layer of atmosphere. The principal research efforts are directed to the development of new stochastic models and simulation technique for solving high-dimensional problems of mathematical physics concentrated around the two main topics which are deeply related via the inner need of stochastic description.

1. Development of new Random Walk methods for solving classical boundary value problems of high dimension not admitting conventional probabilistic representations which is known as an extremely challenging problem in stochastic analysis. Important examples are the static elasticity problems, diffraction and Maxwell equations, and system of nonlinear elliptic equations governing combustion processes.

2. Development of stochastic models and Monte Carlo simulation technique for transport processes in stochastic and turbulent flows. The field of interest includes the transport in the turbulent atmosphere, in rivers, and in porous media. General challenging problem is to determine the area of applicability of classical transport equations based on heuristical closure assumptions, and suggest an alternative stochastic Lagrangian model free of those restrictions. Important features of stochastic Lagrangian methods are the grid free structure, and convenience for solving high-dimensional applied problems like the Footprint problem in the forest environment studies, and the admixture transport in water and soil. Construction of stochastic particles methods and PDF technique (Probability Density Function technique) for simulation of high-dimensional flows governing by linear and nonlinear PDE's involving stochastic parameters like random coefficients, sources, boundaries or boundary conditions. Important examples are the combustion, nucleation and aggregation-disaggregation processes governing by the nonlinear Smoluchowski equation.

## **1. Development of new Random Walk methods for solving classical boundary value problems of high dimension.**

In many interesting boundary value problems the geometry of the domain is extremely complicated, and this is one of the main motivations for the development of the grid free methods, e.g., particle and smoothed particle methods. In stochastic simulation, there are two popular techniques of this kind: (1) the Random Walk methods based on the probabilistic representation of the solutions in the form of an expectation over random diffusion processes, and (2) PDF method which exploits the fact that joint pdf of the state of the system satisfies some PDEs. However both methods have strong restrictions: the first is known only for classical scalar PDEs, and becomes unefficient near the boundary because it is forced to make the integration step smaller and smaller. The PDF method is applied to much broader class of problems, including nonlinear problems for the Navier-Stokes equation, but it cannot be considered as a rigorous method because it describes the processes in the framework of one-particle-fixed time-distributions and involves therefore some semi-empirical closure assumptions.

The Random Walk methods which are based on the Monte Carlo solution of the equivalent integral equations present another class of methods which provide rigorous (i.e., with estimation of the accuracy) numerical solution of linear and non-linear equations [19], [20]. There are two different classes of Random Walk methods: the Walk on Boundary methods, and the Walk inside the domain. The random Walk on Boundary methods are in a sense stochastic counterparts of the boundary element methods [21]. The method is grid free, and uses random points on the boundary. We are developing such methods for different second-order parabolic and elliptic equations, and system of elliptic equations. What is very important, in contrast to the conventional probabilistic representations, in this method all the boundary conditions are possible, and the exterior problems are solved by the same random walk on boundary process. In the class of Random Walk inside the domain, we develop new versions of the Walk on spheres method which enables to solve system of elliptic equations, for instance, the Lamé equation governing the static elasticity processes. In some sense this is a stochastic version of the Schwarz alternative procedure, but the numerical efficiency is much higher for problems of high dimension. We intend to find convergent stochastic algorithms for solving the Lamé equation for a broad class of two and three-dimensional domains [23].

In a cooperation with the group of professor M. Mascagni (Florida State University, Tallahassee, USA), the permeability for a complicated geometry

of a porous medium is studied to find the distribution of the velocity field. The methods used are the Decentred Random Walk on Spheres (DRWS) suggested by K. Sabelfeld and I. Shalimova [23]. In a cooperation with the Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk, an additional validation of the model based on the DRWS method is made by applying the Random Walk on Boundary process.

## **2. Development of stochastic models and Monte Carlo simulation technique for transport of passive scalars and interacting particles in stochastic and turbulent flows.**

Turbulent dispersion of a contaminant, for example pollutant dispersion in the atmosphere, is conveniently described in terms of Lagrangian statistics sampled along the paths of fluid particles [14]. In practice, however, the Eulerian statistics sampled at fixed points in space are better known from experiments. Hence the basic problem of turbulent dispersion is to calculate Lagrangian statistics from given Eulerian statistics. Lagrangian stochastic (LS) models of turbulent dispersion address the problem by statistically characterizing particle paths from an Eulerian input. LS models formulate the time evolution of the particle coordinate and velocity in terms of stochastic differential equations. The LS models are best understood for the description of one-particle statistics, which contain only one-point statistical information and hence lack any information about the different scales of turbulent eddies. A modelled ensemble of single particles allows the calculation of mean concentrations, whereas an ensemble of particle pairs allows the calculation of concentration fluctuations. When we consider the motion of a pair particles, the modelling can be seen as the superposition of a relative motion and the motion of single particle, or particle centroid (e.g., see [28], [26], [25], [27]). The relative motion reflects more directly the internal turbulent structure, because of the appearance of an internal lengths (particle distance), and its description permits the introduction of concepts developed within the theory of turbulence [14].

In the project we deal with one- and two-particle Lagrangian stochastic models for two-dimensional (2D) and three-dimensional (3D) turbulent transport. Here we treat the flow in the Atmospheric Boundary Layer as a fully developed turbulence (i.e., a flow with very high Reynolds number) and consider it as a random velocity field  $(u, v, w)$  which is assumed to be incompressible. Therefore, the trajectories of particles in such flows are stochastic processes. To simulate these stochastic processes, two different approaches

are known in the literature. The first one is based on the numerical solution of the system of random motion equations

$$\frac{\partial X}{\partial t} = u(X, Y, Z, t), \quad \frac{\partial Y}{\partial t} = v(X, Y, Z, t), \quad \frac{\partial Z}{\partial t} = w(X, Y, Z, t).$$

Here  $X(t), Y(t), Z(t)$  are the coordinates of the Lagrangian trajectory at the time  $t$ . The random fields  $u, v, w$  are simulated by Monte Carlo methods (e.g., see [19]), [24], [8], [5]) and the random trajectories are then obtained by numerical solution of the motion equations with the relevant initial data.

In the second approach the true trajectory  $X(t), Y(t), Z(t)$  is assumed to be approximated by a model trajectory  $\hat{X}(t), \hat{Y}(t), \hat{Z}(t)$ , a solution to a stochastic differential equation of Ito type (e.g., see [28], [18], [30], [26], [25]):

$$\begin{aligned} d\hat{X} &= \hat{U}dt, & d\hat{Y} &= \hat{V}dt, & d\hat{Z} &= \hat{W}dt, \\ d\hat{U} &= a_u dt + b_u dB_u(t), & d\hat{V} &= a_v dt + b_v dB_v(t), \\ d\hat{W} &= a_w dt + b_w dB_w(t). \end{aligned}$$

Here we denote by  $\hat{U}, \hat{V}, \hat{W}$  the components of the model Lagrangian velocity,  $B_u(t), B_v(t), B_w(t)$  are three standard independent Wiener processes;  $a_u, a_v, a_w$  and  $b_u, b_v, b_w$  are functions of  $(t, \hat{X}, \hat{Y}, \hat{Z}, \hat{U}, \hat{V}, \hat{W})$ , in general.

It should be noted that in the one-dimensional case, the well-mixed condition uniquely defines the LS model even for non-Gaussian  $p_E$  [28]. In multi-dimensional case, the *uniqueness problem* can be formulated as follows: give physically plausible assumptions which define uniquely the model.

Note that standard LS models deal with quite general inhomogeneous turbulent flows. It is therefore difficult to formulate physically motivated assumptions which, together with the well-mixed condition uniquely define the LS model. Therefore it is reasonable to consider special classes of turbulent flows (e.g., horizontally homogeneous) whose specific features can be used to construct uniquely the LS models under assumptions with credible physical basis.

This is our principal *Ansatz* which we use in constructing new unique LS models, and which enables us to derive the model published in BLM [9]. This uniquely defined Lagrangian stochastic model in the class of well-mixed models is constructed from physically plausible assumptions: (i) in the neutrally stratified horizontally homogeneous surface layer, the vertical motion is mainly controlled by eddies whose size is of order of the current height, and (ii), the streamwise drift term is independent of the crosswind velocity fluctuations. The supposition (i) is motivated by the well known

property that the vertical motion of vortices whose size is much larger than the current height is damped by the ground surface. Therefore, it is reasonable to assume that the vertical drift term is the same as in the isotropic case:  $a'_w = a'_w(t, z, w)$ . As to the point (ii), it comes from the assumption that in the special coordinate system where the  $X$ -axis is oriented along the mean velocity vector, the crosswind velocity fluctuations are symmetrically distributed with respect to the plane  $XZ$ . Different LS models were successively used to solve the Footprint problem [11], [12], [17], and combustion problems [16].

In the free convective layer the mean velocity vector vanishes, and the horizontal motion is isotropic. This property is used to define uniquely the model using only the point (i) of the Assumption. We plan to generalize this approach to other stratifications, in particular, to the difficult case of stable conditions.

### Footprint problem

One field where the stochastic Lagrangian models are very efficiently applied is the Footprint problem.

When carrying out micrometeorological measurements of various scalar surface fluxes, for instance,  $\text{CO}_2$  flux from vegetation, evaporation of fertiliser volatilisation the following problems arise: since the fluxes are given as a correlation between the velocity and concentration of the constituent considered, the sensor cannot be placed too close to the ground for many reasons, in particular, the wind speed is there very small and the size of the measurement instruments is comparable to the length scale of the small eddies near the ground. In addition, near the surface you are in the roughness layer, where you cannot use the typical atmospheric surface layer parametrisations.

The higher the measurement point is placed, the weaker is the signal from the ground, since more of the vertical surface flux is converted into a mean horizontal flux by advection. Also as the measurement height is increased, the sensor "observes" more of the upwind area. Thus if the sensor is placed above a field which abuts on a forest (in the upwind direction), some part of the measurement flux might stem from the forest and not from the field. The analysis of the elevated measurements is also pertinent to inferring surface fluxes from aircraft measurement. The problem is now twofold: how much weaker is the signal in the measurement height and how does the upwind area contribute to the flux in the measurement point. Footprint analysis is the discipline of modeling the fraction of the surface flux (for a given upwind

area) that reaches the sensor. This is rather young research area which has only been the subject of investigation for the past ten years. Footprint analysis made for horizontally homogeneous areas give an estimate of how long homogeneous fetch is needed to make the assumption of horizontal homogeneity valid. The analysis can be used for quantifying the reliability of measurements. One might think also of a footprint analysis before an erection of a mast for several possible positions in order to find "the best" sitting for the mast.

We develop stochastic models and codes for the evaluation of concentration and flux footprint functions. Parametrisation of the surface layer of atmosphere and comparison with the experimental measurements are made in cooperation with Helsinki and Bayreuth universities.

### **Turbulence simulation of the river flow.**

In the model presented the Eulerian pdf  $p_E$  may be not Gaussian, as, for instance, in the forest canopy [4]. It is believed that the model proposed is well suited for the case of neutrally (or close to neutrally) stratified surface layer, which is one of the interesting tasks. One example is the simulation of the turbulent flow in a river we are undertaking in cooperation with the Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, [2].

The effect of turbulence on aquatic photosynthetic organisms transported by river flow is generally associated with two distinctive scales. On a river depth scale (large scale), the turbulence mixing determines the dynamics of light supply to the suspended algae. The algae cells experience a fluctuating intensity and spectral composition of light due to its exponential, wave-length dependent decline with distance from the free surface of flow. At a given light dosage, the intensity of mixing in the vertical plane influences the rate of photosynthesis, the inhibitory effects of UV and algae growth rate. The algae size varies broadly from the size of an individual cell to the size of large colonies or aggregates. On a scale of aggregates (small scale), the shear stresses control the rate of aggregation for algae colonies and their disruption. Maximum size of aggregates is limited by a characteristic micro-scale of river turbulence, Kolmogorov's scale, the scale at which hydrodynamic stresses could torn aggregates to pieces. Thus, properties of environment represented by turbulent flow play critical role in the development of biological processes.

The Langevin-type model developed in the joint paper "On characteristic scales of transport and mixing processes in rivers", by A. Sukhodolov, O. Kurbanmuradov, C. Engelhardt and K. Sabelfeld (see [2]) will be extended

to more general boundary conditions.

### **Transport in porous media.**

The study, prediction, and computation of the transport of particles within a porous medium advected by laminar or turbulent flows is a very challenging problem with broad applicability in many environmental and industrial areas [1], [3]. In addition, understanding flows through porous media is crucial to the efficient and environmental recovery of petrochemicals and other mineral resources, a problem crucial to the economic future of the Europe.

Physically, the problem of flow through porous media includes an enormously wide range of spatial and temporal scales. The extremely high spatial heterogeneity makes conventional deterministic numerical methods practically ineffective. If one considers, for example, only the deterministic computation of even slightly turbulent flow in a porous medium the computational resources required to perform a direct numerical simulation exceed those available on even the most powerful and advanced of today's parallel supercomputers.

Therefore, a probabilistic numerical approach, which requires fewer computational resources, is quite natural as many of the parameters of the porous medium including the permeability, porosity, and hydraulic conductivity can be effectively modeled as random space functions. The flow through such a stochastically parameterized medium is hence itself also a random velocity field.

Many of the problems of interest have, in addition, interacting particles moving within the flows. A good example are problems of colloid formation and related issues of colloid stability and transport in porous medium. These advected particles can interact chemically or through coagulation (aggregation) and disaggregation, so that the particle sizes range from monomers to large polymer clusters. The nonlinear processes of aggregation/disaggregation are governed by the Smoluchowski equation which has an elegant probabilistic interpretation. Hence, it is natural to consider using probabilistic models for the particle transformation and transport thus further motivating the construction of unified Monte Carlo algorithms for both the particle-particle and particle-fluid interactions.

In the porous media transport, only one type of stochastic models was used, namely, the random displacement method (RDM) for hydrodynamic dispersion equation. It should be stressed that RDM can be applied only if the displacement covariance tensor is known (e.g., from measurements, or

numerical simulations), and cannot be applied if the functionals of interest are evaluated at times comparable with the characteristic correlation scale of the flow. In contrast, the Lagrangian stochastic models based on the tracking particles in a random velocity field extracted from numerical solution of the flow equation (for brevity, we will call this model DSM, the direct simulation method) are free of these limitations, but the computational resources required are vast. Therefore, it is quite suggestive to construct a Langevin type stochastic model which is an approximation to DSM, and is written in the form of a stochastic differential equation for the position and velocity. The basis for the Langevin type approach comes from the Kolmogorov similarity theory of fully developed turbulence saying that the velocity structure tensor is a linear function in time which is universal in the inertial subrange. The linearity is the necessary condition to derive a Langevin type equation to mimic the behaviour of the real Lagrangian trajectories. Therefore, the crucial point is here to study if in the porous media, this kind of linear law can be observed. This problem is studied by the DSM, and detailed numerical simulations and comparisons with the random displacement model should be carried out before we can consider this Langevin-type model to be a powerful instrument for practical calculations.

The work is done in cooperation with ULB, Brussels and FZ Jülich, Institute of Chemistry and Dynamics of the Geosphere, with the following joint paper under the preparation: “A Lagrangian Stochastic Model for the Transport in Statistically Homogeneous Porous Media” by O. Kurbanmuradov, K. Sabelfeld, O. Smidts and H. Vereecken.

### **Aggregation-disaggregation processes.**

There are many different mechanisms that bring two particles to each others: Brownian diffusion, gravitational sedimentation, free molecule collisions, turbulent motion of the host gas, acoustic waves, the density, concentration and temperature gradients, particle electric charges.etc., e.g., see [29]. We deal in our project mainly with the case of coagulation of particles in a fully developed turbulence whose small scale statistical structure is specified by  $\varepsilon$ , the kinetic energy dissipation rate, and  $\nu$ , the kinematic viscosity.

The structure of the coagulation kernel  $k_{ij}$  for different collision regimes is presented, e.g., in [29], which is well developed only in the case when there is no spatial dependence of the functions involved in the coagulation equation.

The Smoluchowski equation in the inhomogeneous case governing the

coagulation of particles dispersed by a velocity field  $\mathbf{v}(t, x)$  reads

$$\frac{\partial n_l(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla n_l(\mathbf{x}, t) = \frac{1}{2} \sum_{i+j=l} k_{ij} n_i n_j - n_l \sum_{i=1}^{\infty} k_{li} n_i,$$

where  $n_l(\mathbf{x}, t)$  is the concentration of clusters of size  $l$ ,  $l = 1, 2, \dots$  at a point  $\mathbf{x}$  at time  $t$ ;  $\mathbf{v}(\mathbf{x}, t)$  is the velocity of the host gas,  $k_{ij} = k_{ij}(\mathbf{x}, t)$  is the coagulation coefficient. It is supposed, that the initial size distribution is given:  $n_l(\mathbf{x}, 0) = n_l^0(\mathbf{x})$ .

Our study of the influence of the turbulence intermittency in [13] has shown that this influence can be very high. This approach will be extended to other particle systems, in particular, to the soot particles, colloids and polymers forming in turbulent flows. The work is planned in cooperation with the Statistical Laboratory, Centre of Mathematical Studies, Cambridge University, UK.

Interesting results can be obtained for very complex systems where the coagulation and chemical reactions are closely interplaying, e.g., like in the homogeneous Silane thermal decomposition [15], a project made in cooperation with the Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk.

Other important issues are the analysis of the convergence of stochastic particle method and construction of effective methods for solving inhomogeneous Smoluchowski equation in the spirit of the approach we suggested in [7], [6].

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